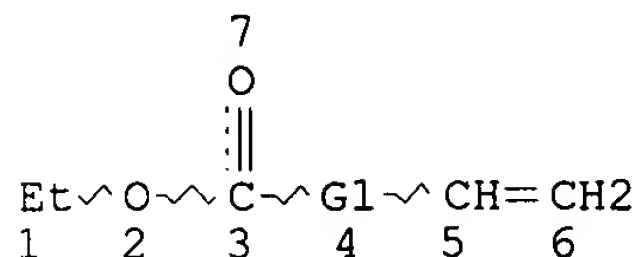


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L14 1 SEA FILE=REGISTRY ABB=ON PLU=ON SILICON/CN  
 L15 1 SEA FILE=REGISTRY ABB=ON PLU=ON 1-DECENE/CN  
 L19 1 SEA FILE=REGISTRY ABB=ON PLU=ON OCTANAL/CN  
 L20 1 SEA FILE=REGISTRY ABB=ON PLU=ON DECANAL/CN  
 L21 1 SEA FILE=REGISTRY ABB=ON PLU=ON "1,7-OCTADIENE"/CN  
 L26 STR

*Considered  
12/10/02 MEZ*



REP G1=(6-10) CH2

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE

L28 2976282 SEA FILE=REGISTRY ABB=ON PLU=ON O=2 AND NC=1  
 L30 5 SEA FILE=REGISTRY SUB=L28 SSS FUL L26  
 L32 4295 SEA FILE=HCAPLUS ABB=ON PLU=ON (L15 OR L19 OR L20 OR L30 OR  
 L21) (L) (RACT OR RCT OR RGT)/RL  
 L36 9 SEA FILE=HCAPLUS ABB=ON PLU=ON L32 AND L14

=&gt; d ibib abs hitstr ind 1-9

L36 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2002:168446 HCAPLUS

DOCUMENT NUMBER: 136:340319

TITLE: Hydride Abstraction Initiated Hydrosilylation of Terminal Alkenes and Alkynes on Porous Silicon

AUTHOR(S): Schmeltzer, J. M.; Porter, Lon A., Jr.; Stewart, Michael P.; Buriak, Jillian M.

CORPORATE SOURCE: Department of Chemistry, 1393 Brown Laboratories, Purdue University, West Lafayette, IN, 47907-1393, USA

SOURCE: Langmuir (2002), 18(8), 2971-2974

CODEN: LANGD5; ISSN: 0743-7463

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

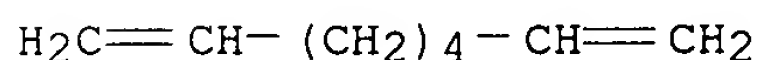
LANGUAGE: English

AB Hydride abstraction by triphenylcarbenium cations in the presence of terminal alkynes and alkenes results in hydrosilylation at room temp. on hydride-terminated porous Si surfaces, leading to alkenyl- and alkyl-terminated surfaces, resp. A wide range of surface terminations are possible as the reaction conditions tolerate a variety of functional groups. Si-C bond formation is substantiated by FTIR and <sup>13</sup>C solid-state NMR spectroscopies, in addn. to chem. and stability studies. Generation of an energetic surface Si-based pos. charge is thus a viable route to the formation of Si-C bonds via hydrosilylation, a step previously postulated

09/803,044

for the mechanism of exciton-mediated hydrosilylation on photoluminescent nanocryst. Si.

IT 3710-30-3, 1,7-Octadiene  
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); **RCT (Reactant)**; PROC (Process); **RACT (Reactant or reagent)**  
 (reaction with silicon surface silylenium; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)  
 RN 3710-30-3 HCAPLUS  
 CN 1,7-Octadiene (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT 7440-21-3, Silicon, reactions  
 RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)  
 (surface functionalization of hydride terminated porous to alkyl and alkenyl terminated; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)  
 RN 7440-21-3 HCAPLUS  
 CN Silicon (7CI, 8CI, 9CI) (CA INDEX NAME)

Si

CC 22-4 (Physical Organic Chemistry)  
 Section cross-reference(s): 6, 29, 57, 58, 73  
 ST alkene hydrosilylation hydride abstraction porous silicon; alkyne hydrosilylation hydride abstraction porous silicon  
 IT NMR (nuclear magnetic resonance)  
 (CP MAS,  $^{13}\text{C}$ ; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)  
 IT IR spectra  
 (FTIR; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)  
 IT Hydroboration  
 (alkenyl terminated silicon surface; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)  
 IT Bond formation  
 (carbon-silicon; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)  
 IT Hydrosilylation  
 Molecular vibration  
 (hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)  
 IT Carbocations  
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)  
 (hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)  
 IT Abstraction reaction  
 (hydride; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)

- IT Luminescence  
(mechanism exciton mediated hydrosilylation of nanocryst. Si and; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)
- IT Exciton  
(mechanism exciton-mediated hydrosilylation on photoluminescent nanocryst. Si and; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)
- IT Cations  
(mechanistic reaction intermediate silylenium; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)
- IT Carbocations  
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)  
(mechanistic reaction intermediate .beta.-silyl; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)
- IT Supramolecular structure  
(nanocryst. Si; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)
- IT Surface treatment  
(org. functionalization; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)
- IT Surface  
(org. modification; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)
- IT Alkenes, reactions  
Alkynes  
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)  
(silicon surface silylenium reaction with terminal; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)
- IT Bond  
(silicon-carbon; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)
- IT NMR spectroscopy  
(solid state, <sup>13</sup>C; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)
- IT Functional groups  
(surface; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)
- IT 7664-39-3, Hydrogen fluoride, reactions  
RL: RCT (Reactant); RGT (Reagent); RACT (Reactant or reagent)  
(etchant; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)
- IT 100-42-5D, Styrene, reaction product with silicon surface silylenium  
592-41-6D, 1-Hexene, reaction product with silicon surface silylenium  
765-03-7D, 1-Dodecyne, ethanolic alk. hydrolysis of hydroboration product  
3710-30-3D, 1,7-Octadiene, reaction product with silicon surface silylenium  
14267-92-6D, 5-Chloro-1-pentyne, reaction product with silicon surface silylenium  
25291-17-2D, 3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluoro-1-octene, reaction product with silicon surface silylenium  
65909-92-4D, 1,7-Octenyne, reaction product with silicon surface silylenium

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)  
 (hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)

IT 341-02-6, Trityl tetrafluoroborate  
 RL: RCT (Reactant); RGT (Reagent); RACT (Reactant or reagent)  
 (hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)

IT 627-19-0D, 1-Pentyne, reaction product with silicon surface silylenium  
 RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)  
 (hydroboration; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)

IT 28149-31-7D, Silylenium, silicon surface tied  
 RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)  
 (mechanistic reaction intermediate; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)

IT 100-42-5, Styrene, reactions 592-41-6, 1-Hexene, reactions 627-19-0, 1-Pentyne 765-03-7, 1-Dodecyne 3710-30-3, 1,7-Octadiene 14267-92-6, 5-Chloro-1-pentyne 25291-17-2, 3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluoro-1-octene 65909-92-4, 1,7-Octenyne  
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); **RCT (Reactant)**; PROC (Process); **RACT (Reactant or reagent)**  
 (reaction with silicon surface silylenium; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)

IT 7440-21-3, Silicon, reactions  
 RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)  
 (surface functionalization of hydride terminated porous to alkyl and alkenyl terminated; hydride abstraction initiated hydrosilylation of terminal alkenes and alkynes on porous silicon)

REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER (2) OF 9 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:728692 HCAPLUS

DOCUMENT NUMBER: 136:25655

TITLE: Derivatization of porous silicon nanostructures with functional 1-alkenes and non-conjugated dienes

AUTHOR(S): Boukherroub, Rabah; Wayner, Danial D. M.; Lockwood, David J.; Canham, Leigh T.

CORPORATE SOURCE: Steacie Institute for Molecular Sciences, National Research Council, Ottawa, ON, K1A 0R6, Can.

SOURCE: Proceedings - Electrochemical Society (2001), 2000-25(Pits and Pores II: Formation, Properties, and Significance for Advanced Materials), 586-601  
 CODEN: PESODO; ISSN: 0161-6374

PUBLISHER: Electrochemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Freshly prepd. porous Si (PSi) surfaces were modified with different org. mols. such as alkenes (1-decene, Et undecylenate) and nonconjugated dienes (1,7-octadiene) in a thermal process to yield org. monolayers covalently

*this invention*

attached to the surface through Si-C bonds. These monolayers were characterized using diffuse reflectance IR Fourier transform (DRIFT), x-ray photoelectron and Raman spectroscopies. Derivatized surfaces showed a high stability in boiling aq. and org. solvents, and in 49% HF and KOH (pH = 13) solns. at room temp. They protect the surface against oxidn. when exposed to air at 100% humidity. The high passivation of the surface implies also photoluminescence (PL) stabilization. In fact, the modified surfaces retained their original PL, and the chem. process affected neither the peak position nor the intensity. The PL was preserved even after a steam treatment for several weeks while the H terminated porous layer was completely transformed into a transparent oxide.

IT 7440-21-3, Silicon, properties

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(derivatization of porous silicon nanostructures with functional 1-alkenes and non-conjugated dienes)

RN 7440-21-3 HCAPLUS

CN Silicon (7CI, 8CI, 9CI) (CA INDEX NAME)

Si

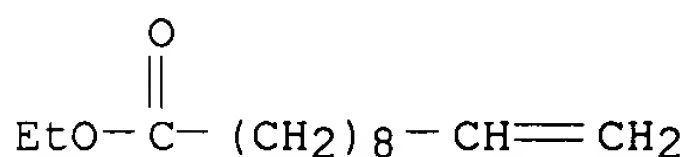
IT 692-86-4 872-05-9, 1-Decene 3710-30-3,  
1,7-Octadiene

RL: RCT (Reactant); RACT (Reactant or reagent)

(derivatization of porous silicon nanostructures with functional 1-alkenes and non-conjugated dienes)

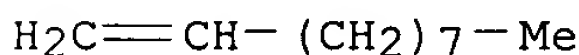
RN 692-86-4 HCAPLUS

CN 10-Undecenoic acid, ethyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



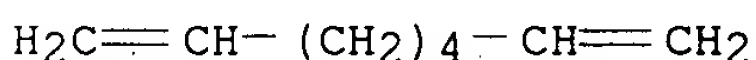
RN 872-05-9 HCAPLUS

CN 1-Decene (8CI, 9CI) (CA INDEX NAME)



RN 3710-30-3 HCAPLUS

CN 1,7-Octadiene (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 66-3 (Surface Chemistry and Colloids)

Section cross-reference(s): 67

ST derivatization porous silicon nanostructure alkene nonconjugated diene reaction

IT Nanostructures

(derivatization of porous silicon nanostructures with functional 1-alkenes and non-conjugated dienes)

IT Stability  
(of monolayers of functional alkenes and non-conjugated dienes on derivatized porous silicon surfaces)

IT Passivation  
(of porous silicon nanostructures using functional alkenes and non-conjugated dienes in relation to photoluminescence)

IT Luminescence  
(passivation of porous silicon nanostructures using functional alkenes and non-conjugated dienes in relation to photoluminescence)

IT Oxidation  
(surface; protection the surface against oxidn. using functional alkenes and non-conjugated dienes in derivatization of porous silicon nanostructures)

IT 7440-21-3, Silicon, properties  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)  
(derivatization of porous silicon nanostructures with functional 1-alkenes and non-conjugated dienes)

IT 692-86-4 872-05-9, 1-Decene 3710-30-3, 1,7-Octadiene  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(derivatization of porous silicon nanostructures with functional 1-alkenes and non-conjugated dienes)

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:510737 HCAPLUS

DOCUMENT NUMBER: 135:233748

TITLE: Exciton-Mediated Hydrosilylation on Photoluminescent Nanocrystalline Silicon

AUTHOR(S): Stewart, Michael P.; Buriak, Jillian M.

CORPORATE SOURCE: Department of Chemistry, Purdue University, West Lafayette, IN, 47907-1393, USA

SOURCE: Journal of the American Chemical Society (2001), 123(32), 7821-7830  
CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A novel white light-promoted reaction using photoluminescent nanocryst. silicon enables the hydrosilylation of alkenes and alkynes, providing stabilization of the porous silicon without significant loss of the photoemissive qualities of the material. Photopatterning and lithog. fabrication of isolated porous silicon structures are made possible. Expts. and observations are presented which indicate that the light promoted hydrosilylation reaction is unique to photoluminescent silicon, and does not function on nonemissive material. Hydrosilylation using a reactive center generated from a surface-localized exciton is proposed based upon exptl. evidence, explaining the photoluminescence requirement. Indirect excitons formed by light absorption mediate the formation of localized electrophilic surface states which are attacked by incoming alkene or alkyne nucleophiles. Supra-band gap charge carriers have sufficient energy to react with nucleophilic alkenes and alkynes,



thereupon causing Si-C bond formation, an irreversible event. The light-promoted hydrosilylation reaction is quenched by reagents that quench the light emission from porous silicon, via both charge transfer and energy transfer pathways.

IT 872-05-9, 1-Decene

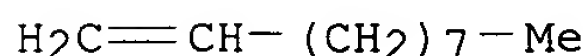
RL: PEP (Physical, engineering or chemical process); PRP (Properties);

RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(exciton-mediated hydrosilylation of alkenes and alkynes on hydride-terminated porous silica and formation of C-Si bonds in relation to photolithog.)

RN 872-05-9 HCAPLUS

CN 1-Decene (8CI, 9CI) (CA INDEX NAME)



IT 7440-21-3, Silicon, properties

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(porous; exciton-mediated hydrosilylation of alkenes and alkynes on hydride-terminated porous silica and formation of C-Si bonds in relation to photolithog.)

RN 7440-21-3 HCAPLUS

CN Silicon (7CI, 8CI, 9CI) (CA INDEX NAME)

Si

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

ST exciton mediated hydrosilylation alkene alkyne photoluminescent nanocryst silicon; photolithog photolytic hydrosilylation alkene alkyne photoluminescent nanocryst silicon

IT Exciton

Luminescent substances

Surface photolysis

(exciton-mediated hydrosilylation of alkenes and alkynes on hydride-terminated porous silica and formation of C-Si bonds in relation to photolithog.)

IT Alkenes, reactions

Alkynes

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(exciton-mediated hydrosilylation of alkenes and alkynes on hydride-terminated porous silica and formation of C-Si bonds in relation to photolithog.)

IT Luminescence

(luminescence of derivatized surfaces prepd. by exciton-mediated hydrosilylation of alkenes and alkynes on hydride-terminated porous silica in relation to photolithog.)

IT Hydrosilylation

(photochem.; exciton-mediated hydrosilylation of alkenes and alkynes on hydride-terminated porous silica and formation of C-Si bonds in relation to photolithog.)

IT Electron transfer

- Energy transfer  
IR spectra  
(photolytic hydrosilylation of alkenes and alkynes on  
hydride-terminated porous silica quenched by)
- IT Charge transfer complexes  
RL: PEP (Physical, engineering or chemical process); PRP (Properties);  
PROC (Process)  
(photolytic hydrosilylation of alkenes and alkynes on  
hydride-terminated porous silica quenched by)
- IT Photolithography  
(photopatterning based on exciton-mediated hydrosilylation of alkenes  
and alkynes on hydride-terminated porous silica and formation of C-Si  
bonds)
- IT 7440-36-0, Antimony, uses 7440-42-8, Boron, uses 7723-14-0,  
Phosphorus, uses  
RL: MOA (Modifier or additive use); USES (Uses)  
(exciton-mediated hydrosilylation of alkenes and alkynes on  
hydride-terminated porous silica and formation of C-Si bonds in  
relation to photolithog.)
- IT 100-42-5, Styrene, reactions 111-78-4, 1,5-Cyclooctadiene 112-41-4,  
1-Dodecene 536-74-3, Phenylacetylene 592-41-6, 1-Hexene, reactions  
627-19-0, 1-Pentyne 629-05-0, 1-Octyne 765-03-7, 1-Dodecyne  
766-97-2, 4-Methylphenylacetylene 871-84-1, 1,7-Octadiyne  
872-05-9, 1-Decene 873-73-4, 4-Chlorophenylacetylene  
6089-09-4, 4-Pentynoic acid 14918-21-9, 5-Hexynenitrile 21652-58-4,  
1H,1H,2H-Perfluorodecene 25291-17-2 26256-87-1, Tri(ethylene glycol)  
methyl vinyl ether 99685-96-8, Fullerene  
RL: PEP (Physical, engineering or chemical process); PRP (Properties);  
**RCT (Reactant)**; PROC (Process); **RACT (Reactant or reagent)**  
(exciton-mediated hydrosilylation of alkenes and alkynes on  
hydride-terminated porous silica and formation of C-Si bonds in  
relation to photolithog.)
- IT 1873-77-4, Tris(trimethylsilyl)silane  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(photolysis of tris(trimethylsilyl)silane and pentyne in relation to  
exciton-mediated hydrosilylation of alkenes and alkynes on  
hydride-terminated porous silica)
- IT 7440-21-3, Silicon, properties  
RL: PEP (Physical, engineering or chemical process); PRP (Properties);  
PROC (Process)  
(porous; exciton-mediated hydrosilylation of alkenes and alkynes on  
hydride-terminated porous silica and formation of C-Si bonds in  
relation to photolithog.)
- IT 102-54-5, Ferrocene 781-43-1, 9,10-Dimethylantracene 1271-51-8,  
Vinylferrocene 1273-89-8, Ethylferrocene 1287-13-4, Ruthenocene  
1499-10-1, 9,10-Diphenylantracene 84821-53-4, Decamethylruthenocene  
RL: PEP (Physical, engineering or chemical process); PRP (Properties);  
PROC (Process)  
(quencher; photolytic hydrosilylation of alkenes and alkynes on  
hydride-terminated porous silica quenched by)

REFERENCE COUNT: 102 THERE ARE 102 CITED REFERENCES AVAILABLE FOR  
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT

L36 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2002 ACS  
ACCESSION NUMBER: 2001:435186 HCAPLUS  
DOCUMENT NUMBER: 135:55020



TITLE: Substituted phthalocyanines and their precursors  
 INVENTOR(S): Cook, Michael John; Heeney, Martin James  
 PATENT ASSIGNEE(S): ~~Gentian AS, Norway~~  
 SOURCE: PCT Int. Appl., 146 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001042368	A1	20010614	WO 2000-GB4708	20001208
<p>W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM</p> <p>RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG</p>				
EP 1238016	A1	20020911	EP 2000-985506	20001208
<p>R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR</p>				
NO 2002002663	A	20020808	NO 2002-2663	20020605
PRIORITY APPLN. INFO.:				
			GB 1999-29064	A 19991208
			GB 2000-12348	A 20000522
			GB 2000-25817	A 20001020
			WO 2000-GB4708	W 20001208

OTHER SOURCE(S): MARPAT 135:55020

AB Process is claimed for the prepn. of metal phthalocyanines and their precursors including phthalonitrile sulfonate esters, substituted phthalonitriles and substituted phthalocyanines, phthalonitrile halides. For example 3,6-didecylphthalonitrile was prepd. from 3,6-bis(trifluoromethanesulfonyloxy)phthalonitrile and decylzinc iodide and reacted with 4,5-dibromo-3,6-dibutoxyphthalonitrile, prepd. from bromination of 2,3-dicyanohydroquinone, in presence of Ni(OAc)<sub>2</sub>·4H<sub>2</sub>O to give [1,4-dibutoxy-2,3-dibromo-8,11,15,18,22,25-hexadecylphthalocyaninato]nickel. The metal phthalocyanine derivs. have applications as photosensitizers for use in photodynamic therapy.

IT 7440-21-3D, Silicon, phthalocyanine deriv. complexes, biological studies

RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(as photosensitizers and for use in photodynamic therapy)

RN 7440-21-3 HCAPLUS

CN Silicon (7CI, 8CI, 9CI) (CA INDEX NAME)

Si

IT 872-05-9, 1-Decene

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant for prepn. of metal phthalocyanine complexes for use in photodynamic therapy and as photosensitizers)

RN 872-05-9 HCAPLUS  
CN 1-Decene (8CI, 9CI) (CA INDEX NAME)

$\text{H}_2\text{C}=\text{CH}-(\text{CH}_2)_7-\text{Me}$

IC ICM C09B047-067  
ICS C09B047-04; C07D487-22; A61K041-00; C07D487-22; C07D259-00;  
C07D209-00; C07D209-00; C07D209-00; C07D209-00  
CC 78-7 (Inorganic Chemicals and Reactions)  
Section cross-reference(s): 8, 28, 63, 74  
ST phthalocyanine metal complex prepn photodynamic therapy photosensitizer;  
phthalonitrile sulfonate ester substituted prepn  
IT Keratosis  
(actinic)  
IT Prostate gland  
(benign hyperplasia; metal phthalocyanine complexes for treatment of)  
IT Mycosis  
(fungoides, inhibitors; metal phthalocyanine complexes as)  
IT Artery, disease  
(intima, hyperplasia; metal phthalocyanine complexes for treatment of)  
IT Mouth  
(lichen planus)  
IT Antiarthritics  
Antibacterial agents  
Antitumor agents  
Antiviral agents  
Fungicides  
(metal phthalocyanine complexes as)  
IT Peptides, uses  
Polyanhydrides  
Polyesters, uses  
Polyoxyalkylenes, uses  
Polyphosphazenes  
RL: NUU (Other use, unclassified); USES (Uses)  
(metal phthalocyanine complexes embedded in polymer for use in  
photodynamic therapy or as photosensitizers)  
IT Atherosclerosis  
Eczema  
Hemophilia  
Hyperplasia  
Prion diseases  
Psoriasis  
(metal phthalocyanine complexes for treatment of)  
IT Skin, neoplasm  
(mycosis fungoides, inhibitors; metal phthalocyanine complexes as)  
IT Antitumor agents  
(mycosis fungoides; metal phthalocyanine complexes as)  
IT Luminescence  
Quantum transition  
(of metal phthalocyanine complexes as photosensitizers and use in  
photodynamic therapy)  
IT Rare earth complexes  
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES  
(Uses)  
(phthalocyanine; as photosensitizers and for use in photodynamic

- therapy)
- IT Transition metal complexes  
 RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (phthalocyanine; prepn. of metal phthalocyanine complexes for use in photodynamic therapy and as photosensitizers)
- IT Metallophthalocyanines  
 RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. for use in photodynamic therapy and as photosensitizers)
- IT Photosensitizers (pharmaceutical)  
 (prepn. of metallophthalocyanines as)
- IT Photodynamic therapy  
 (prepn. of metallophthalocyanines for use in)
- IT Metallophthalocyanines  
 RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)  
 (rare earth complexes; as photosensitizers and for use in photodynamic therapy)
- IT Artery, disease  
 (restenosis; metal phthalocyanine complexes for treatment of)
- IT Artery, disease  
 (stenosis; metal phthalocyanine complexes for treatment of)
- IT Metallophthalocyanines  
 RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (transition metal complexes; prepn. of metal phthalocyanine complexes for use in photodynamic therapy and as photosensitizers)
- IT 7429-90-5D, Aluminum, phthalocyanine deriv. complexes, biological studies  
 7439-89-6D, Iron, phthalocyanine deriv. complexes, biological studies  
 7439-92-1D, Lead, phthalocyanine deriv. complexes, biological studies  
 7439-95-4D, Magnesium, phthalocyanine deriv. complexes, biological studies  
 7440-02-0D, Nickel, phthalocyanine deriv. complexes, biological studies  
 7440-03-1D, Niobium, phthalocyanine deriv. complexes, biological studies  
 7440-05-3D, Palladium, phthalocyanine deriv. complexes, biological studies  
 7440-06-4D, Platinum, phthalocyanine deriv. complexes, biological studies  
**7440-21-3D**, Silicon, phthalocyanine deriv. complexes, biological studies  
 7440-31-5D, Tin, phthalocyanine deriv. complexes, biological studies  
 7440-48-4D, Cobalt, phthalocyanine deriv. complexes, biological studies  
 7440-50-8D, Copper, phthalocyanine deriv. complexes, biological studies  
 7440-55-3D, Gallium, phthalocyanine deriv. complexes, biological studies  
 7440-56-4D, Germanium, phthalocyanine deriv. complexes, biological studies  
 7440-62-2D, Vanadium, phthalocyanine deriv. complexes, biological studies  
 7440-66-6D, Zinc, phthalocyanine deriv. complexes, biological studies  
 7440-70-2D, Calcium, phthalocyanine deriv. complexes, biological studies  
 7440-74-6D, Indium, phthalocyanine deriv. complexes, biological studies  
 RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)  
 (as photosensitizers and for use in photodynamic therapy)
- IT 7440-66-6P, Zinc, preparation  
 RL: PUR (Purification or recovery); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)  
 (dust; or prepn. of metal phthalocyanine complexes as photosensitizers and use in photodynamic therapy)
- IT 311-28-4, Tetrabutylammonium iodide 603-35-0, Triphenylphosphine, uses  
 7647-10-1, Palladium dichloride 13965-03-2,

Dichlorobis(triphenylphosphine)palladium 14221-01-3,  
Tetrakis(triphenylphosphine)palladium 14264-16-5,  
Dichlorobis(triphenylphosphine)nickel 51364-51-3, Pd2(dba)3  
RL: CAT (Catalyst use); USES (Uses)  
(for prepn. of metal phthalocyanine complexes for use in photodynamic  
therapy and as photosensitizers)

IT 9003-39-8, Polyvinylpyrrolidone 21442-01-3, N-(2-  
Hydroxypropyl)methacrylamide 25322-68-3, Poly(ethylene glycol)  
RL: NUU (Other use, unclassified); USES (Uses)  
(metal phthalocyanine complexes embedded in polymer for use in  
photodynamic therapy or as photosensitizers)

IT 162978-27-0 336854-52-5 344454-06-4  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
study, unclassified); BIOL (Biological study)  
(photosensitized inactivation of human fibroblasts by)

IT 288303-39-9P 320614-48-0P 320614-51-5P 344453-47-0P 344453-49-2P  
344453-50-5P 344453-51-6P 344453-54-9P 344453-55-0P 344453-57-2P  
344453-61-8P 344453-62-9P 344453-67-4P  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN  
(Synthetic preparation); PREP (Preparation); PROC (Process)  
(prepn. and photophysics)

IT 344453-56-1P 344453-59-4P  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT  
(Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC  
(Process); RACT (Reactant or reagent)  
(prepn. and photophysics and demetalation)

IT 320614-32-2P  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT  
(Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC  
(Process); RACT (Reactant or reagent)  
(prepn. and photophysics and deprotection)

IT 344453-66-3P  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT  
(Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC  
(Process); RACT (Reactant or reagent)  
(prepn. and photophysics and reaction with methylbutynol)

IT 288303-38-8P 320614-36-6P  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT  
(Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC  
(Process); RACT (Reactant or reagent)  
(prepn. and photophysics and reaction with trimethylsilylacetylene)

IT 200056-52-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and reactant for prepn. of metal phthalocyanine complexes as  
photosensitizers and use in photodynamic therapy)

IT 4593-01-5P, 4,5-Dibromo-3,6-dihydroxyphthalonitrile 181219-01-2P  
288303-40-2P, 4,5-Dibromo-3,6-dibutoxyphthalonitrile 320614-40-2P,  
4-Bromo-3,6-dibutoxyphthalonitrile 344453-68-5P 344453-69-6P  
344453-70-9P 344453-71-0P 344453-72-1P 344453-73-2P 344453-74-3P  
344453-75-4P 344453-76-5P 344453-77-6P 344453-78-7P 344453-79-8P  
344453-80-1P 344453-81-2P 344454-04-2P 344454-05-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and reactant for prepn. of metal phthalocyanine complexes for  
use in photodynamic therapy and as photosensitizers)

IT 138497-25-3P

RL: BYP (Byproduct); PREP (Preparation)  
(prepn. of)

IT 344453-48-1P 344453-52-7P 344453-53-8P 344453-58-3P 344453-60-7P  
344453-63-0P 344453-64-1P 344453-65-2P 344453-82-3P 344453-83-4P  
344453-84-5P 344453-85-6P 344453-86-7P 344453-87-8P 344453-91-4P  
344453-92-5P 344453-95-8P 344453-96-9P 344453-97-0P 344453-98-1P  
344454-03-1P 344570-54-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

IT 344453-88-9P 344453-89-0P 344453-90-3P 344453-93-6P 344453-94-7P  
344453-99-2P 344454-00-8P 344454-01-9P 344454-02-0P

RL: BUU (Biological use, unclassified); PEP (Physical, engineering or  
chemical process); PRP (Properties); SPN (Synthetic preparation); BIOL  
(Biological study); PREP (Preparation); PROC (Process); USES (Uses)  
(prepn. of metal phthalocyanine complexes for use in photodynamic  
therapy and as photosensitizers)

IT 344453-20-9P

RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL  
(Biological study); PREP (Preparation); USES (Uses)  
(reactant for prepn. of metal phthalocyanine complexes as  
photosensitizers and use in photodynamic therapy)

IT 288-32-4, Imidazole, reactions 358-23-6, Trifluoromethanesulfonic  
anhydride 375-72-4, Nonafluorobutanesulfonyl fluoride 1018-79-7,  
2,3-Dicyano-1,4-dihydroxynaphthalene 2050-77-3, 1-Iododecane  
4733-50-0, 2,3-Dicyanohydroquinone 131379-39-0 135579-83-8  
155589-48-3 344453-19-6

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reactant for prepn. of metal phthalocyanine complexes as  
photosensitizers and use in photodynamic therapy)

IT 36360-42-6P, 3,6-Diphenylphthalonitrile 344453-21-0P 344453-22-1P  
344453-27-6P 344453-29-8P 344453-31-2P 344453-32-3P 344453-33-4P  
344453-34-5P 344453-35-6P 344453-36-7P 344453-37-8P 344453-38-9P  
344453-39-0P 344453-40-3P 344453-41-4P 344453-42-5P 344453-43-6P  
344453-44-7P 344453-45-8P 344453-46-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(reactant for prepn. of metal phthalocyanine complexes as  
photosensitizers and use in photodynamic therapy)

IT 119931-48-5P, 3,6-Didecylphthalonitrile 344453-24-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(reactant for prepn. of metal phthalocyanine complexes as  
photosensitizers and use in photodynamic therapy)

IT 98-80-6, Phenylboronic acid 110-89-4, Piperidine, reactions 112-55-0,  
1-Dodecanethiol 115-19-5, 2-Methyl-3-butyn-2-ol 124-63-0,  
Methanesulfonyl chloride 301-04-2, Lead diacetate 629-05-0, 1-Octyne  
688-74-4, Tributoxyboron 872-05-9, 1-Decene 994-89-8,  
Tributyl(ethynyl)tin 1066-54-2, Trimethylsilylacetylene 3282-30-2,  
Pivaloyl chloride 5720-07-0, 4-Methoxyphenylboronic acid 5970-45-6,  
Zinc acetate dihydrate 6018-89-9, Nickel diacetate tetrahydrate  
6165-68-0, 2-Thiopheneboronic acid 7699-45-8, Zinc bromide 7786-30-3,  
Magnesium chloride, reactions 10025-82-8, Indium trichloride  
10365-98-7, 3-Methoxyphenylboronic acid 14047-29-1, p-  
Carboxyphenylboronic acid 15854-87-2, 4-Iodopyridine 18869-47-1,  
DL-Tyrosine methyl ester 28611-39-4, 4-Dimethylaminophenylboronic acid  
59016-93-2, 4-(Hydroxymethyl)phenylboronic acid 89343-06-6,  
Triisopropylsilylacetylene 89415-43-0, p-Aminophenylboronic acid  
92511-12-1 189068-39-1



RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant for prepn. of metal phthalocyanine complexes for use in photodynamic therapy and as photosensitizers)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:315870 HCAPLUS

DOCUMENT NUMBER: 135:67993

TITLE: Ideal Passivation of Luminescent Porous Silicon by Thermal, Noncatalytic Reaction with Alkenes and Aldehydes

AUTHOR(S): Boukherroub, R.; Morin, S.; Wayner, D. D. M.; Bensebaa, F.; Sproule, G. I.; Baribeau, J.-M.; Lockwood, D. J.

CORPORATE SOURCE: Steacie Institute for Molecular Sciences Institute for Chemical Process and Environmental Technology and Institute for Microstructural Sciences, National Research Council of Canada, Ottawa, ON, K1A 0R6, Can.

SOURCE: Chemistry of Materials ~~(2001)~~, 13(6), 2002-2011  
CODEN: CMATEX; ISSN: 0897-4756

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB This paper describes the chem. modification of high surface area, photoluminescent porous Si (PSi) by reaction at a moderately elevated temp. (<115.degree.) with alkenes (RCH:CH<sub>2</sub>) and aldehydes (RCHO) to give org. monolayers covalently bonded to the surface through Si-C and Si-O-C linkages, resp. The monolayers are characterized using diffuse reflectance IR Fourier transform (DRIFT), transmission FTIR, Raman, x-ray photoelectron, and Auger spectroscopies. Auger depth profiling results are consistent with homogeneous incorporation of org. mols. on the internal surface of the PSi. The functionalized surfaces demonstrate high chem. stability in boiling aq. and org. solvents and even in harsher environments such as aq. HF or KOH. Aging in ambient air for several months has no effect on the PL intensity or energy. Notably, when the surfaces were treated at 100% humidity at 70.degree. for 6 wk, only a small increase in the PL intensity was obsd. This severe treatment completely transformed H-terminated PSi into a transparent oxide layer. This result is consistent with the formation of org. films with a very low defect d. at the interface. Thus, these org. monolayers have unprecedented stability and ideally passivate the PSi.

IT 112-31-2, Decylaldehyde 124-13-0, Octylaldehyde  
872-05-9, 1-Decene

RL: RCT (Reactant); RACT (Reactant or reagent)

(ideal passivation of luminescent porous silicon by thermal, noncatalytic reaction with alkenes and aldehydes)

RN 112-31-2 HCAPLUS

CN Decanal (8CI, 9CI) (CA INDEX NAME)

OHC-(CH<sub>2</sub>)<sub>8</sub>-Me

RN 124-13-0 HCAPLUS

CN Octanal (8CI, 9CI) (CA INDEX NAME)



OHC-(CH<sub>2</sub>)<sub>6</sub>-Me

RN 872-05-9 HCAPLUS  
CN 1-Decene (8CI, 9CI) (CA INDEX NAME)

H<sub>2</sub>C=CH-(CH<sub>2</sub>)<sub>7</sub>-Me

IT 7440-21-3, Silicon, properties  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); TEM  
(Technical or engineered material use); PROC (Process); USES (Uses)  
(porous; ideal passivation of luminescent porous silicon by thermal,  
noncatalytic reaction with alkenes and aldehydes)  
RN 7440-21-3 HCAPLUS  
CN Silicon (7CI, 8CI, 9CI) (CA INDEX NAME)

Si

CC 73-5 (Optical, Electron, and Mass Spectroscopy and Other Related  
Properties)  
ST passivation luminescence porous silicon alkene aldehyde noncatalytic  
reaction  
IT Interfacial structure  
(AFM images; cross section of luminescent porous silicon)  
IT IR reflectance spectra  
(diffuse; of luminescent porous silicon passivated by thermal,  
noncatalytic reaction with alkenes and aldehydes)  
IT Passivation  
(ideal passivation of luminescent porous silicon by thermal,  
noncatalytic reaction with alkenes and aldehydes)  
IT Aldehydes, reactions  
Alkenes, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(ideal passivation of luminescent porous silicon by thermal,  
noncatalytic reaction with alkenes and aldehydes)  
IT Luminescence  
Raman spectra  
X-ray spectra  
(of luminescent porous silicon passivated by thermal, noncatalytic  
reaction with alkenes and aldehydes)  
IT X-ray reflectivity spectra  
(of pure and H-terminated porous silicon)  
IT 112-31-2, Decylaldehyde 124-13-0, Octylaldehyde  
872-05-9, 1-Decene  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(ideal passivation of luminescent porous silicon by thermal,  
noncatalytic reaction with alkenes and aldehydes)  
IT 7440-21-3, Silicon, properties  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); TEM  
(Technical or engineered material use); PROC (Process); USES (Uses)  
(porous; ideal passivation of luminescent porous silicon by thermal,  
noncatalytic reaction with alkenes and aldehydes)

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:516399 HCAPLUS

DOCUMENT NUMBER: 131:132136

TITLE: Acidic mesoporous catalysts

INVENTOR(S): Yahav, Ganapati Dadasaheb; Krishnan, M. S.; Doshi,  
Nirav Shashikant; Purjari, Ajit Atmaram; Rahuman, M.  
S. M. Mujeebur

PATENT ASSIGNEE(S): Secretary Department of Science and Technology, India

SOURCE: Brit. UK Pat. Appl., 34 pp.

CODEN: BAXXDU

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2332155	A1	19990616	GB 1998-27396	19981211
GB 2332155	B2	20010912		
JP 2000042416	A2	20000215	JP 1998-375450	19981214
US 6204424	B1	20010320	US 1998-211499	19981214
PRIORITY APPLN. INFO.:			IN 1997-DE3590 A	19971212
			IN 1997-DE3594 A	19971212
			IN 1997-DE3595 A	19971212

OTHER SOURCE(S): MARPAT 131:132136

AB An eco-friendly synergistic heterogeneous solid catalyst for use in reactions, such as alkylation, oligomerization, isomerization, hydration, dehydration, etherification, esterification, hydrocracking, and nitration of org. compds., comprises synergistic combination of sulfated metal oxide and mesoporous zeotypes comprising Si 50-60, Zr 40-50, and S 5-10 wt.%, and having surface area of 200-500 m<sup>2</sup>/g, pore vol. of 0.1-0.3 m<sup>3</sup>/g, pore diam. of 25-35 .ANG., and XRD peak at 20 being 0-3. The invention also covers the process of manuf. of the above catalysts and its use in particular for producing oligomers from .alpha.-olefins, Friedel-Crafts alkylation and acylation reactions.

IT 7440-21-3, Silicon, uses

RL: CAT (Catalyst use); USES (Uses)

(catalysts contg.; acidic mesoporous catalysts for alkylation and oligomerization)

RN 7440-21-3 HCAPLUS

CN Silicon (7CI, 8CI, 9CI) (CA INDEX NAME)

Si

IT 872-05-9, 1-Decene

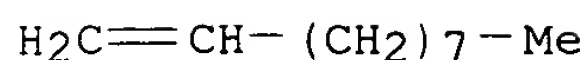
RL: RCT (Reactant); RACT (Reactant or reagent)

(dimerization; acidic mesoporous catalysts)

RN 872-05-9 HCAPLUS

CN 1-Decene (8CI, 9CI) (CA INDEX NAME)

H<sub>2</sub>C=CH-(CH<sub>2</sub>)<sub>7</sub>-Me



IC ICM B01J035-10  
ICS B01J027-053; C07C002-16; C07C029-00

CC 51-11 (Fossil Fuels, Derivatives, and Related Products)  
Section cross-reference(s): 45, 67

ST acidic mesoporous catalyst; oligomerization catalyst acidic mesoporous olefin oligomer; Friedel Crafts alkylation acylation acidic mesoporous catalyst

IT Alkenes, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(C6-12 .alpha.-; acidic mesoporous catalysts for alkylation and oligomerization)

IT Alkylation catalysts  
Dimerization catalysts  
Friedel-Crafts reaction catalysts  
(acidic mesoporous catalysts for alkylation and oligomerization)

IT Zeolites (synthetic), uses  
RL: CAT (Catalyst use); USES (Uses)  
(acidic mesoporous catalysts for alkylation and oligomerization)

IT Petroleum refining catalysts  
(alkylation; acidic mesoporous catalysts for alkylation and oligomerization)

IT Molecular sieves  
(mesoporous; acidic mesoporous catalysts for alkylation and oligomerization)

IT Polymerization catalysts  
(oligomerization; acidic mesoporous catalysts for alkylation and oligomerization)

IT 17438-89-0P, 1-Decene dimer  
RL: PNU (Preparation, unclassified); PREP (Preparation)  
(acidic mesoporous catalysts)

IT 101-81-5P, Diphenylmethane 27776-01-8P  
RL: PNU (Preparation, unclassified); PREP (Preparation)  
(acidic mesoporous catalysts for Friedel-Crafts alkylation)

IT 100-44-7, Benzyl chloride, reactions 108-88-3, Toluene, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(acidic mesoporous catalysts for Friedel-Crafts alkylation)

IT 71-43-2, Benzene, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(acidic mesoporous catalysts for acylation)

IT 122-01-0, 4-Chlorobenzoyl chloride  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(acidic mesoporous catalysts for acylation of benzene with)

IT 134-85-0P, 4-Chlorobenzophenone  
RL: PNU (Preparation, unclassified); PREP (Preparation)  
(acidic mesoporous catalysts for acylation of benzene with 4-chlorobenzoyl chloride)

IT 769-92-6P, 4-tert-Butylaniline 2409-55-4P, 2-tert-Butyl-p-cresol  
RL: PNU (Preparation, unclassified); PREP (Preparation)  
(acidic mesoporous catalysts for alkylation)

IT 62-53-3, Benzenamine, reactions 75-65-0, reactions 106-44-5, reactions 1634-04-4, MTBE  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(acidic mesoporous catalysts for alkylation)

IT 7699-43-6, Zirconium oxychloride

RL: CAT (Catalyst use); USES (Uses)  
 (acidic mesoporous catalysts for alkylation and oligomerization)

IT 18602-27-2P, 1-Octene dimer  
 RL: PNU (Preparation, unclassified); PREP (Preparation)  
 (acidic mesoporous catalysts for prepn. of)

IT 17438-89-ODP, 1-Decene dimer, hydrogenated  
 RL: PNU (Preparation, unclassified); PREP (Preparation)  
 (as lubricants; acidic mesoporous catalysts for prepn. of)

IT 1314-23-4D, Zirconia, sulfated 7429-90-5, Aluminum, uses 7439-89-6,  
 Iron, uses 7440-21-3, Silicon, uses 7440-31-5, Tin, uses  
 7440-32-6, Titanium, uses 7440-67-7, Zirconium, uses 7440-69-9,  
 Bismuth, uses 14808-79-8, Sulfate, uses  
 RL: CAT (Catalyst use); USES (Uses)  
 (catalysts contg.; acidic mesoporous catalysts for alkylation and  
 oligomerization)

IT 872-05-9, 1-Decene  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (dimerization; acidic mesoporous catalysts)

IT 7446-09-5, Sulfur dioxide, uses 7446-11-9, Sulfur trioxide, uses  
 7664-93-9, Sulfuric acid, uses 7783-06-4, Hydrogen sulfide, uses  
 7783-20-2, Ammonium sulfate, uses  
 RL: NUU (Other use, unclassified); RCT (Reactant); RACT (Reactant or  
 reagent); USES (Uses)  
 (sulfating agent; in prepn. of acidic mesoporous catalysts for  
 alkylation and oligomerization)

L36 .ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:16013 HCAPLUS

DOCUMENT NUMBER: 130:144567

TITLE: Alkyl-terminated Si(111) surfaces: A high-resolution,  
 core level photoelectron spectroscopy study

AUTHOR(S): Terry, Jeff; Linford, Matthew R.; Wigren, Christer;  
 Cao, Renyu; Pianetta, Piero; Chidsey, Christopher E.  
 D.

CORPORATE SOURCE: Stanford University, Stanford, CA, 94309, USA

SOURCE: Journal of Applied Physics (1999), 85(1), 213-221

CODEN: JAPIAU; ISSN: 0021-8979

PUBLISHER: American Institute of Physics

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The bonding of alkyl monolayers to Si(111) surfaces has been studied with  
 high-resoln. core level photoelectron spectroscopy (PES). Two very  
 different wet-chem. methods have been used to prep. the alkyl monolayers:  
 (i) Olefin insertion into the H-Si bond of the H-Si(111) surface, and (ii)  
 replacement of Cl on the Cl-Si(111) surface by an alkyl group from an  
 alkyllithium reagent. In both cases, PES has revealed a C 1s component  
 shifted to lower binding energy and a Si 2p component shifted to higher  
 binding energy. Both components are attributed to the presence of a C-Si  
 bond at the interface. Along with photoelectron diffraction data [Appl.  
 Phys. Lett. 71, 1056, (1997)], these data are used to show that these two  
 synthetic methods can be used to functionalize the Si(111) surface.

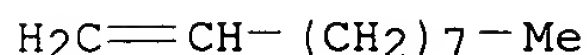
IT 872-05-9, 1-Decene

RL: RCT (Reactant); RACT (Reactant or reagent)

(alkyl-terminated silicon prepd. by Olefin insertion of 1-alkenes into  
 the H-Si bond of the H-Si(111) surface, and replacement of Cl on the  
 Cl-Si(111) surface by an alkyl group from an alkyllithium reagent)

RN 872-05-9 HCAPLUS

CN 1-Decene (8CI, 9CI) (CA INDEX NAME)



IT 7440-21-3, Silicon, properties  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties);  
 PROC (Process)  
 (hydrogen-, chlorine-, alkyl-terminated; bonding of alkyl monolayers to  
 Si(111) surfaces studied with high-resoln. core level photoelectron  
 spectroscopy)

RN 7440-21-3 HCAPLUS

CN Silicon (7CI, 8CI, 9CI) (CA INDEX NAME)

Si

CC 66-4 (Surface Chemistry and Colloids)

Section cross-reference(s): 22, 73

ST alkyl terminated silicon surface photoelectron spectroscopy; passivation  
 chlorine hydrogen terminated silicon

IT Annealing  
 (annealing alkyl monolayers to Si(111) surfaces studied with  
 high-resoln. core level photoelectron spectroscopy)

IT Adsorbed monolayers  
 Alkyl groups  
 Chemical chains  
 (bonding of alkyl monolayers to Si(111) surfaces studied with  
 high-resoln. core level photoelectron spectroscopy)

IT Passivation  
 (novel alkyl passivation monolayers on Si(111) surfaces studied with  
 high-resoln. core level photoelectron spectroscopy)

IT 2229-07-4D, Methyl, reaction prodn. with Si surface 2492-36-6D, Butyl,  
 reaction prodn. with Si surface 2672-01-7D, Pentyl, reaction prodn. with  
 Si surface 34448-85-6D, Octadecyl, reaction prodn. with Si surface  
 49765-51-7D, Decyl, reaction prodn. with Si surface  
 RL: MOA (Modifier or additive use); PRP (Properties); USES (Uses)  
 (alkyl-terminated silicon prepd. by Olefin insertion into the H-Si bond  
 of the H-Si(111) surface, and replacement of Cl on the Cl-Si(111)  
 surface by an alkyl group from an alkyllithium reagent)

IT 12385-13-6, Hydrogen atomic, reactions 22537-15-1, Chlorine atomic,  
 reactions  
 RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or  
 reagent); USES (Uses)

(alkyl-terminated silicon prepd. by Olefin insertion into the H-Si bond  
 of the H-Si(111) surface, and replacement of Cl on the Cl-Si(111)  
 surface by an alkyl group from an alkyllithium reagent)

IT 109-72-8, Butyllithium, reactions 917-54-4, Methyllithium

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (alkyl-terminated silicon prepd. by Olefin insertion into the H-Si bond  
 of the H-Si(111) surface, and replacement of Cl on the Cl-Si(111)  
 surface by an alkyl group from an alkyllithium reagent)

IT 109-67-1, 1-Pentene 112-88-9, 1-Octadecene 872-05-9, 1-Decene

RL: **RCT (Reactant); RACT (Reactant or reagent)**  
 (alkyl-terminated silicon prepd. by Olefin insertion of 1-alkenes into

the H-Si bond of the H-Si(111) surface, and replacement of Cl on the Cl-Si(111) surface by an alkyl group from an alkyllithium reagent)

IT 7440-21-3, Silicon, properties  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties);  
 PROC (Process)  
 (hydrogen-, chlorine-, alkyl-terminated; bonding of alkyl monolayers to Si(111) surfaces studied with high-resoln. core level photoelectron spectroscopy)

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1997:780864 HCAPLUS  
 DOCUMENT NUMBER: 128:132889  
 TITLE: Reactivity of the H-Si (111) surface  
 AUTHOR(S): Terry, Jeff; Mo, Renee; Wigren, Christer; Cao, Renyu; Mount, George; Pianetta, Piero; Linford, Matthew R.; Chidsey, Christopher E.D.  
 CORPORATE SOURCE: Stanford Synchrotron Radiation Laboratory, Stanford Linear Accelerator Center, Stanford, CA, USA  
 SOURCE: Nuclear Instruments & Methods in Physics Research, Section B: Beam Interactions with Materials and Atoms (1997), 133(1-4), 94-101  
 CODEN: NIMBEU; ISSN: 0168-583X  
 PUBLISHER: Elsevier Science B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB H-Si (111) surfaces exposed to Cl<sub>2</sub>, Br<sub>2</sub>, and 1-alkenes were studied with photoemission spectroscopy. These particular compds. were chosen because of their importance in semiconductor processing and surface functionalization. The observation of the growth of a Si 2p component at high binding energy, characteristic of halogen reactivity, confirmed that Br and Cl gases both reacted with the H-Si (111) surface. Reactions with 1-alkenes were confirmed by measuring both the Si 2p and the C 1s core level spectra. The C 2s-based MOs in the valence band revealed the identity of the alkyl monolayer on the Si (111) surface. Therefore, the H-Si (111) surface, under certain conditions, was reactive.

IT 872-05-9, 1-Decene 7440-21-3, Silicon, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reactivity of hydrogen-silicon (111) surface)

RN 872-05-9 HCAPLUS  
 CN 1-Decene (8CI, 9CI) (CA INDEX NAME)

H<sub>2</sub>C=CH-(CH<sub>2</sub>)<sub>7</sub>-Me

RN 7440-21-3 HCAPLUS  
 CN Silicon (7CI, 8CI, 9CI) (CA INDEX NAME)

Si

CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)  
 Section cross-reference(s): 66  
 ST surface reactivity hydrogenated silicon; chlorination hydrogenated silicon



surface; bromination hydrogenated silicon surface; alkylation hydrogenated silicon surface

IT Alkylation  
Bromination  
Chlorination  
Halogenation  
(reactivity of hydrogen-silicon (111) surface)

IT Alkenes, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reactivity of hydrogen-silicon (111) surface)

IT Reactivity (chemical)  
(surface; reactivity of hydrogen-silicon (111) surface)

IT 1333-74-0, Hydrogen, uses  
RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)  
(reactivity of hydrogen-silicon (111) surface)

IT 109-67-1, 1-Pentene 112-88-9, 1-Octadecene **872-05-9**, 1-Decene  
**7440-21-3**, Silicon, reactions 7726-95-6, Bromine, reactions  
7782-50-5, Chlorine, reactions  
RL: **RCT (Reactant); RACT (Reactant or reagent)**  
(reactivity of hydrogen-silicon (111) surface)

L36 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1993:106144 HCAPLUS

DOCUMENT NUMBER: 118:106144

TITLE: Catalytic oligomerization process using synthetic mesoporous crystalline material

INVENTOR(S): Bhore, Nazeer A.; Le, Quang N.; Yokomizo, Grant H.

PATENT ASSIGNEE(S): Mobil Oil Corp., USA

SOURCE: U.S., 16 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5134243	A	19920728	US 1991-718893	19910621
WO 9300165	A1	19930107	WO 1992-US4864	19920610
W: AU, CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE				
AU 9222364	A1	19930125	AU 1992-22364	19920610
AU 654201	B2	19941027		
EP 579776	A1	19940126	EP 1992-914476	19920610
EP 579776	B1	19990120		
R: BE, DE, FR, GB, IT, NL				
JP 06509071	T2	19941013	JP 1992-501505	19920610
JP 3110043	B2	20001120	JP 1993-501505	19920610
US 5260501	A	19931109	US 1992-920944	19920728

PRIORITY APPLN. INFO.: US 1991-718879 A 19910621  
US 1991-718884 A 19910621  
US 1991-718893 A 19910621  
WO 1992-US4864 A 19920610

AB A process for upgrading olefins employs a synthetic catalyst for ultra-large pore cryst. material. The cryst. material exhibits unusually large sorption capacity demonstrated by its benzene adsorption capacity of

.gtorsim.15 g benzene/100 g at 50 torr and 25.degree., a hexagonal electron diffraction pattern that can be indexed with a d100 value .gtorsim.18 .ANG. and a hexagonal arrangement of uniformly sized pores with a max. perpendicular cross section of .gtorsim.13 .ANG. units. The process for catalytic oligomerization of olefin feedstock comprises contacting the feedstock with acid metallocosilicate solid catalyst having the structure of MCM-41 with hexagonal honeycomb lattice structure consisting essentially of uniform pores of 20-100 .ANG.. The oligomerization reaction is selective, esp. when conducted at 40-250.degree.. Low severity reaction permits conversion of lower olefins at 100-13,000 pKa and moderate space velocity.

IT **7440-21-3**, Silicon, uses  
 RL: CAT (Catalyst use); USES (Uses)  
 (catalysts contg., zeolites, ultra-large pore, for olefin oligomerization)  
 RN 7440-21-3 HCAPLUS  
 CN Silicon (7CI, 8CI, 9CI) (CA INDEX NAME)

Si

IT **872-05-9**, 1-Decene  
 RL: **RCT (Reactant); RACT (Reactant or reagent)**  
 (oligomerization of, zeolite MCM 41 catalyst for, with ultra-large pores, for synthetic lubricants)  
 RN 872-05-9 HCAPLUS  
 CN 1-Decene (8CI, 9CI) (CA INDEX NAME)

$\text{H}_2\text{C}=\text{CH}-(\text{CH}_2)_7-\text{Me}$

IC ICM C07C002-12  
 NCL 585533000  
 CC 51-6 (Fossil Fuels, Derivatives, and Related Products)  
 Section cross-reference(s): 45  
 ST olefin oligomerization catalyst MCM 41  
 IT Alkenes, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (C3-5, oligomerization of, zeolite MCM 41 catalyst for, with ultra-large pores)  
 IT Zeolites, uses  
 RL: CAT (Catalyst use); USES (Uses)  
 (MCM 41, catalysts, with ultra-large pores, for oligomerization)  
 IT Petroleum refining catalysts  
 (oligomerization, zeolite MCM 41, with ultra-large pores, for gasoline and diesel fuel components and synthetic lubricants)  
 IT 7429-90-5, Aluminum, uses 7439-89-6, Iron, uses 7439-95-4, Magnesium, uses **7440-21-3**, Silicon, uses 7440-42-8, Boron, uses 7440-55-3, Gallium, uses 7440-56-4, Germanium, uses 7723-14-0, Phosphorus, uses  
 RL: CAT (Catalyst use); USES (Uses)  
 (catalysts contg., zeolites, ultra-large pore, for olefin oligomerization)  
 IT 115-07-1, 1-Propene, uses  
 RL: RCT (Reactant); RACT (Reactant or reagent)

(oligomerization of, zeolite MCM 41 catalyst for, with ultra-large pores)

IT 872-05-9, 1-Decene

RL: RCT (Reactant); RACT (Reactant or reagent)

(oligomerization of, zeolite MCM 41 catalyst for, with ultra-large pores, for synthetic lubricants)